

Quantum Espresso 6.8

Webpage

<https://www.quantum-espresso.org/>

Version

6.8

Build Environment

- Intel Parallel Studio 2018 update 4

Files Required

- q-e-qe-6.8.tar.gz

Build Procedure

```
#!/bin/sh

VERSION=6.8
BASEDIR=/home/users/${USER}/Software/QE/${VERSION}
TARBALL=${BASEDIR}/q-e-qe-${VERSION}.tar.gz

INSTDIR=/local/apl/lx/espresso68
PARALLEL=12

# -----
umask 0022

module purge
module load intel_parallelstudio/2018update4

export LANG=C
export LC_ALL=C
ulimit -s unlimited

cd ${INSTDIR}
if [ -d q-e-qe-${VERSION} ]; then
  mv q-e-qe-${VERSION} q-e-qe-erase
  rm -rf q-e-qe-erase &
fi

tar xzf ${TARBALL}
mv q-e-qe-${VERSION}/* .
mv q-e-qe-${VERSION}/.[a-z]* .
rmdir q-e-qe-${VERSION}

export MPIF90=mpiifort
export MPIFC=mpiifort
export MPIF77=mpiifort
export MPICC=mpiicc
export MPICXX=mpiicpc

FC=ifort F90=ifort F77=ifort CC=icc CXX=icpc \
FFLAGS="-O3 -assume byterecl -ip -g" \
./configure --enable-parallel --with-scalapack=intel

# pwall(pw neb ph pp pwcond acfdt) cp ld1 tddfpt hp xspectra gw1
echo "==== all ===="
make -j${PARALLEL} all
```

```
echo "==== all_currents ===="
make -j${PARALLEL} all_currents

for i in epw w90 couple; do
  echo "==== $i ===="
  make -j${PARALLEL} $i
done

for i in yambo; do
  echo "==== $i ===="
  make $i
done

cd test-suite
make run-tests-serial
make clean
make run-tests-parallel
cd ..
```

Notes

- passed all the tests.
- d3q is not enabled (compilation error)
 - (it maybe possible to compile by loading rand() function correctly.)
- intel2020 failed as in [the previous \(6.7\) case](#).
- gfortran doesn't work well.
 - binaries built with versions 6, 8 didn't work
 - binaries built with ver 9, 10 failed on some of tests
 - other versions were not tested.